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# The ground state and vortices in a two-dimensional Bose gas confined in a harmonic trap

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## Abstract

We study the ground state properties of a two-dimensional Bose gas in an harmonic trap potential using the recently proposed mean-field equation that takes into account the correct dimensionality effect. In contrast to the three-dimensional case, the interaction term depends logarithmically on the scattering length and density. We compare our results with other approaches with various forms for the two-dimensional coupling. We also consider the vortex states and study the effects of density-dependent interactions on the formation of vortices.

## 1. Introduction

The observation of Bose–Einstein condensation (BEC) in externally confined atomic vapours [1] has had a large impetus on the theoretical study of interacting boson systems in general. The thermodynamic, ground-state static and dynamic properties of condensates are extensively investigated and the main results are compiled in a number of review articles [2]. Most of the excitement stems from the possibility of understanding the properties of a macroscopic quantum state. Apart from fundamental physics considerations, the Bose–Einstein condensed systems offer interesting atom laser applications.

The BEC phenomenon in two-dimensional (2D) systems has attracted a considerable amount of interest from the point of view of understanding the effects of dimensionality. As the homogeneous 2D system of bosons would not undergo BEC at a finite temperature, the prospects of observing BEC in systems with an external potential [3] provides a strong motivation for such investigations. It was argued by Mullin [4] that BEC is not possible for strictly 2D systems even in a trapping potential in the thermodynamic limit. However, by varying the trapping field so that it is very narrow in one direction, it should be possible to separate the single-particle states of the oscillator potential into well-defined bands, and occupying the lowest band should produce an effectively 2D system. A growing number of recent experiments [5–10] point to the possibility of realizing quasi-two-dimensional (Q2D) trapped atomic gases, and measurements on the BEC transition temperature and other properties are expected to follow.

The studies on BEC in 2D systems can be broadly divided into two categories. In the first group the interaction effects are treated parametrically without reference to the actual interaction potential or the scattering length which describes it as in the 3D formulation of the interacting boson condensates [11–14]. Included in the same category of calculations researchers have used path integral Monte Carlo simulations [15] at finite temperature to give indications of a BEC transition in 2D systems. In the second group, some effort is made to relate the 2D interaction strength to the 3D scattering length [16–18] or to solve the scattering problem in strictly two dimensions to obtain the relevant dependence of the interaction coupling on the scattering length. Using 2D scattering theory Kim *et al* [19] found that the interaction strength depends logarithmically on the scattering length. In a series of papers Shevchenko [20, 21] studied an interacting 2D Bose gas in a nonuniform field arriving at the conclusion that even though BEC does not take place, the system exhibits superfluidity. Recently, Kolomeisky *et al* [22], in their treatment of low-dimensional Bose liquids, suggested a modified form for the mean-field description of 2D condensates. Lieb *et al* [23] have rigorously analysed this and related approximations as applied to the practical cases of interest. Using scattering theory arguments Petrov *et al* [24] obtained a slightly more detailed form of the effective interaction coupling for Q2D systems that distinguishes different density regimes.

The central aim of this paper is to calculate the ground-state properties of 2D Bose condensates based on the formulation given by Shevchenko [21] and Kolomeisky *et al* [22] and study the effects of density-dependent interaction strength. There are several works that consider Q2D Bose condensates in harmonic trap potentials using a model for the effective interaction strength. In contrast to the strictly 2D problem, the Q2D model takes into account the influence of the transverse direction in terms of the confinement frequency  $\omega_z$ . Recent experiments [5–10] indicate that such realizations will be possible in the near future. In a recent calculation we have provided an assessment of the utility of simplified models compared to the more rigorous form of the equations governing the physics of 2D Bose condensates [25]. We also calculate, in this paper, the vortex state wavefunction for a 2D system and discuss the conditions for the formation of vortices.

The rest of this paper is organized as follows. In the next section, we first discuss the mean-field description of Bose condensates within the local-density approximation. Specializing to the case of 2D bosons in a harmonic trap at zero temperature, we calculate the condensate wavefunction and illustrate the effects of density-dependent interaction. We then look at the vortex state wavefunction in 2D systems and calculate the critical frequency of rotation necessary for the formation of vortices. We conclude with a brief summary.

## 2. Theoretical background

The ground-state properties of a condensed system of bosons at zero temperature are described by the Gross–Pitaevskii (GP) equation [26]. In the presence of external trapping potentials, therefore an inhomogeneous Bose system, it is useful to adopt the local-density approximation which regards the system as being locally homogeneous. The mean-field energy functional in the local-density approximation can, very generally, be written as [27]

$$E = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla\psi|^2 + V_{\text{ext}}(\mathbf{r})|\psi|^2 + \epsilon(\rho)|\psi|^2 \right], \quad (1)$$

where  $\epsilon(\rho)$  is the ground-state energy (per particle) of the homogeneous system and  $\rho = |\psi|^2$  is the density. Variation of the energy functional with respect to  $\psi^*$ , subject to the normalization condition  $\int d\mathbf{r} |\psi|^2 = N$ , yields the nonlinear Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{ext}}(\mathbf{r})\psi + \frac{\partial[\epsilon(\rho)\rho]}{\partial\rho} \psi = \mu\psi, \quad (2)$$

where  $\mu$  is the chemical potential. The local-density approximation was used by Fabrocini and Polls [28] and Nunes [27] to study high-density effects in 3D condensates, by making use of the 3D homogeneous hard-sphere Bose gas results from perturbation theory. These studies showed that the modifications to the GP equation become important as the number of particles  $N$  and the hard-sphere radius  $a$  are increased, making the system less dilute.

We now apply the above scheme to a 2D system of bosons in a harmonic isotropic trapping potential  $V_{\text{ext}}(\mathbf{r}) = m\omega_{\perp}^2 r^2/2$ . Perturbation theory calculations for a homogeneous system of 2D hard-disc bosons yield [29]

$$\epsilon(\rho) = \frac{\hbar^2}{2m} \frac{4\pi\rho}{|\ln \rho a^2|}, \quad (3)$$

for the ground-state energy (per particle). The corresponding mean-field equation for the condensate wavefunction thus reads [22]

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + \frac{1}{2} m\omega_{\perp}^2 r^2 \psi(r) + \frac{\hbar^2}{2m} \frac{8\pi}{|\ln \psi^2 a^2|} |\psi(r)|^2 \psi(r) = \mu\psi. \quad (4)$$

The energy functional corresponding to this equation has also been suggested by Shevchenko [21]. We shall call equation (4) the 2D GP equation, and compare it with other suggested forms to describe the ground state of 2D Bose condensates. We note that equation (4) is quite different to its 3D counterpart, in that the dimensionless interaction term  $g = 1/|\ln \psi^2 a^2|$  not only depends on the hard-disc radius  $a$  logarithmically, but it also depends on  $|\psi|^2$ , making the GP equation highly nonlinear. In three dimensions the density-dependent interactions arise as corrections or modifications to the GP equation, whereas in two dimensions the mean-field interaction is density dependent. Here, we cast the nonlinear term in the form  $\frac{\hbar^2}{2m} g \psi^3$ . In the following we shall present numerical results of the solution of equation (4) and compare them with other approximations.

In the previous applications [27, 28, 30] of the local-density approximation in 3D condensates, effects beyond the mean-field theory (GP equation) have been explored by including higher-order terms in the homogeneous energy density  $\epsilon(\rho)$ . In two dimensions, the correct mean-field description is given by equation (4). To go beyond the mean-field theory one would have to use the higher-order terms in the homogeneous energy density calculation [31]. Another possible correction to the mean-field description has been suggested by Andersen and Haugerud [32]. In their treatment the kinetic energy functional is modified to include a gradient term

$$E_{\text{kin}} = \frac{\hbar^2}{2m} \int d\mathbf{r} \left[ 1 - \frac{2}{3} \frac{1}{|\ln |\psi|^2 a^2|} \right] |\nabla \psi|^2. \quad (5)$$

In our numerical calculations which are presented and discussed in the next section, we have tested the significance of corrections brought by the gradient term. We have found that it has negligible effect on the condensate profile  $\psi(r)$  and other physical quantities for the range of  $N$  and scattering length values we examined.

### 3. Results and discussion

We numerically solve the 2D GP equation given in equation (4) using the steepest descent method [28, 33], which is known to produce accurate results. We also minimize the corresponding energy functional over a set of spline test functions, as performed by Krauth [34]

in his comparison of quantum Monte Carlo simulations with mean-field solutions. In both cases our numerical results are in good agreement. A further check of our numerical calculations is provided by the virial relation. Under the scaling transformation  $\mathbf{r} \rightarrow \alpha \mathbf{r}$ , so that  $\psi(\mathbf{r}) \rightarrow \psi(\mathbf{r})/\alpha$ , and using the variational nature of the energy we obtain

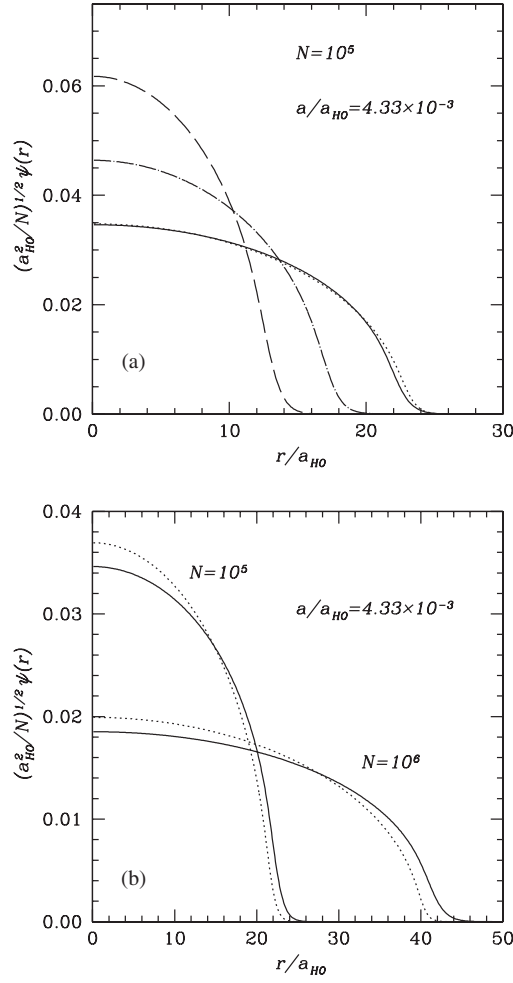
$$E_{\text{kin}} - E_{\text{ext}} + E_{\text{int}} + 2\pi \int d\mathbf{r} \frac{|\psi(\mathbf{r})|^4}{|\ln |\psi|^2 a^2|^2} = 0. \quad (6)$$

In this form of the virial relation, we have omitted the gradient correction to the kinetic energy, since numerically it is found to be negligible. Our solution of the GP equation satisfies the virial relation to a high degree of accuracy.

We now illustrate the ground state wavefunction  $\psi(r)$  obtained by solving the 2D GP equation. In the figures we are going to present, we scale lengths by the harmonic oscillator length  $a_{\text{HO}} = (\hbar/m\omega_{\perp})^{1/2}$ , and energies by  $\hbar\omega_{\perp}$ . We also normalize  $\psi(r)$  for a given number of particles  $N$ . To compare the results of strictly 2D condensates with models taking the transverse direction into account [16, 17], we also consider a model system with interaction strength  $g = \sqrt{2\pi}(a/a_{\text{HO}})\lambda$ , where  $\lambda = \omega_z/\omega_{\perp}$  is the asymmetry parameter. In figure 1 we show the scaled condensate wavefunction  $\psi(r)$  in a 2D harmonic trap as a function of the radial distance. We have chosen  $a/a_{\text{HO}} = 4.33 \times 10^{-3}$ , the s-wave scattering length of  $^{87}\text{Rb}$  atoms, for the hard-disc radius describing the interaction strength. This corresponds to a trap frequency of  $\omega_{\perp}/(2\pi) = 78$  Hz. To see how a constant  $g$  model [16] compares with the 2D GP equation, we present in figure 1(a) the condensate wavefunction  $\psi(r)$  for several values of  $\lambda$ . We find that large values of the asymmetry parameter  $\lambda$  ( $\lambda = 10^4$  in our example) describe the condensate wavefunction quite accurately. Our results show that the strictly 2D limit may be achieved by experimentally tuning the parameter  $\lambda$ . The constant  $g$  approximation will have great utility in modelling the 2D dynamics of Bose condensates in terms of the parameters of the external trapping potentials. The 2D GP equation suggested by Kim *et al* [19] makes use of scattering theory to obtain  $g = |\ln ka|^{-1}$ , where  $k$  is some inverse length scale. This differs from the above constant  $g$  model somewhat, but the correct choice of  $k$  would produce a similar condensate wavefunction for practical purposes.

Recently Lieb *et al* [23] argued that a simplified form of equation (4) would be sufficient for the leading order calculations. They suggested that the logarithmic term should be replaced by  $\ln \bar{\rho} a^2$ , where  $\bar{\rho}$  is the average density, defined by  $\bar{\rho} = \frac{1}{N} \int \rho_1^{\text{TF}}(\mathbf{r})^2 d\mathbf{r}$ . Here,  $\bar{\rho}$  is expressed in terms of an average over  $\rho_1^{\text{TF}}(\mathbf{r})$ , the Thomas–Fermi (TF) density when the logarithmic term is absent. The TF approximation simply neglects the kinetic energy in equation (4) since the interaction term dominates for the most part, except in the region  $\psi(r)$  where it vanishes. For the harmonic trapping potential in two dimensions, we find  $\bar{\rho} a_{\text{HO}}^2 = N^{1/2}/3\pi$ . In figure 1(b) we compare the resulting condensate wavefunction for the proposed  $g \sim |\ln \bar{\rho} a^2|^{-1}$  model. We observe that when equation (4) is used the interaction term has a larger effect and the condensate shows depletion near the centre compared to the approximation suggested by Lieb *et al* [23]. In 2D systems, the dilute limit is characterized by the condition  $\rho a^2/|\ln \rho a^2| \ll 1$ . For our chosen parameters of typical values this condition is fulfilled. It is then interesting to observe the effects of a logarithmic term on the overall shape of the condensate wavefunction.

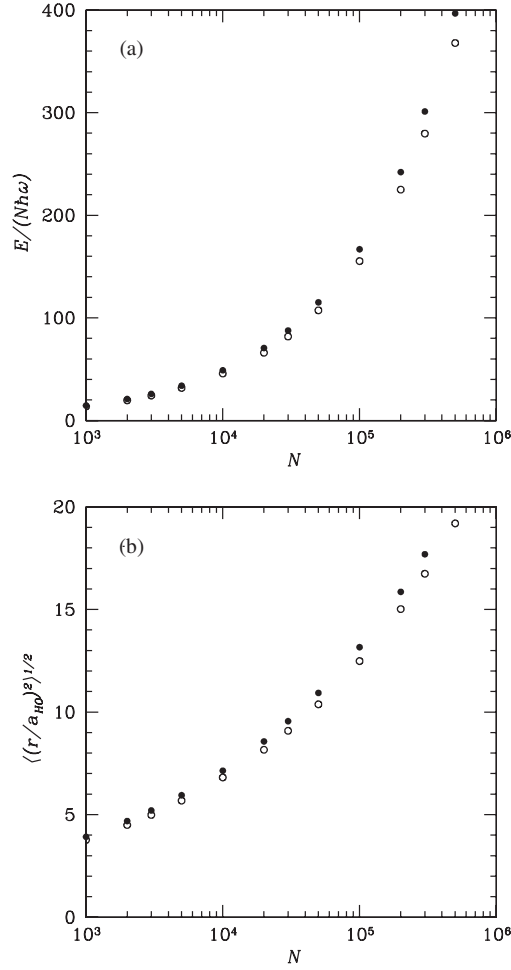
We further elucidate the difference between the results of the full GP equation and the approximation suggested by Lieb *et al* [23] by looking at the ground state energy and root-mean-square value of the radial coordinate. In figure 2(a) we plot the ground state energy (per particle)  $E/N$  as a function of the particle number  $N$  for these two approaches. We note that for small values of  $N$ , i.e.  $N \lesssim 10^4$ , the ground state energies are very close. As  $N$  increases,  $E/N$  starts to reflect the difference between the two approaches. As the approximation proposed by Lieb *et al* [23] has the effect of decreasing the interaction strength  $g$ , we find an increase in the



**Figure 1.** (a) The condensate wavefunction  $\psi(r)$  with  $|\ln \psi^2 a^2|^{-1}$  correction (solid curve) as a function of the radial distance for a system of  $N = 10^5$  atoms and hard-disc radius  $a/a_{HO} = 4.33 \times 10^{-3}$ , compared to that with the constant  $g$  interaction model. The dashed, dot-dashed and dotted curves correspond to the asymmetry parameters  $\lambda = 10^2, 10^3$  and  $10^4$ , respectively. (b) The condensate wavefunction  $\psi(r)$  for systems of  $N = 10^5$  and  $10^6$  atoms. The solid and dotted curves indicate the solutions of the mean-field equation with  $\ln |\psi|^2 a^2$  and  $\ln |\bar{\rho} a^2|$  factors, respectively, as explained in the text.

ground state energy for large  $N$  when the full 2D GP equation is used. Figure 2(b) shows the root mean square value  $\langle r^2 \rangle^{1/2}$  of the radial coordinate as a function of  $N$ . Similar effects are also observed in this case related to the effective interaction strength in respective approaches.

Other approaches [11–14] to describe condensates in two dimensions have used a coupling constant  $g$  treated as a parameter. We have previously discussed [25] the qualitative differences between such models and the present formulation. The interaction term in the local-density approximation-based 2D GP equation does not allow for negative scattering lengths, because of its quadratic dependence on  $a$ . In the Q2D model of Petrov *et al* [24] the attractive mean-field interaction is shown to have a resonant character, namely, becoming repulsive for very large values of  $a_{HO}^z$ . This would mean a large asymmetry parameter  $\lambda = \omega_z/\omega_\perp$  and hence a more 2D-like condensate.



**Figure 2.** (a) The ground state energy as a function of the particle number  $N$ . The solid and empty circles indicate calculations using the mean-field equation with  $\ln |\psi|^2 a^2$  and  $\ln |\bar{\rho} a^2|$  factors, respectively. (b) The root mean square of the radial coordinate  $(r^2)^{1/2}$  as a function of the particle number  $N$ . The solid and empty circles indicate calculations using the mean-field equation with  $\ln |\psi|^2 a^2$  and  $\ln |\bar{\rho} a^2|$  factors, respectively.

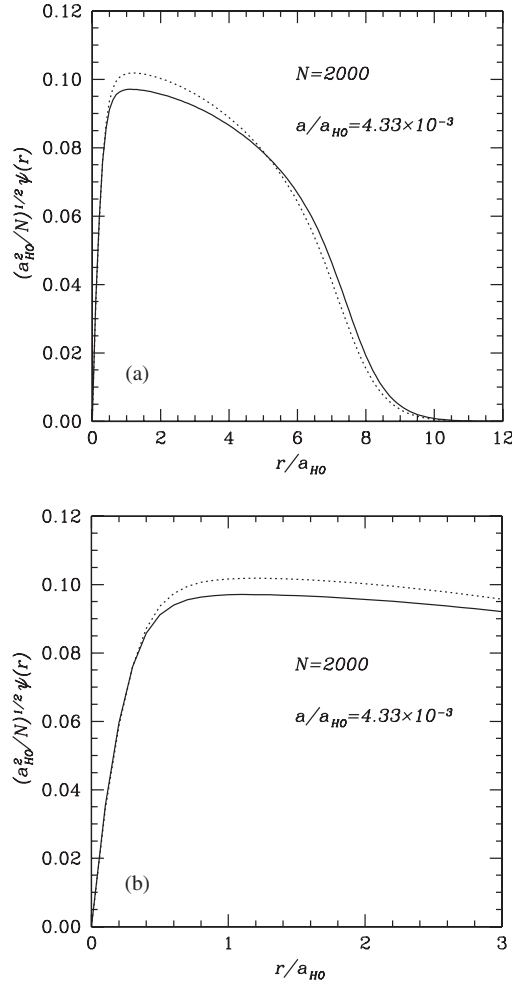
The formalism set out in the previous section to describe the ground-state properties of 2D condensates may be generalized to include vortex states which are of recent theoretical and experimental interest [35, 36]. To describe the condensate with vortices, we introduce a wavefunction of the form

$$\Psi(r) = \psi(r)e^{i\kappa\phi}, \quad (7)$$

where  $\kappa$  is an integer and  $\phi$  is the polar angle. Substituting  $\Psi$  into the GP equation we obtain

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + \frac{\hbar^2\kappa}{2mr^2}\psi(r) + \frac{1}{2}m\omega_{\perp}^2 r^2\psi(r) + \frac{\hbar^2}{2m} \frac{8\pi}{|\ln \psi^2 a^2|} |\psi(r)|^2\psi(r) = \mu\psi(r). \quad (8)$$

Figure 3(a) displays the wavefunction characterizing the vortex ( $\kappa = 1$ ) solution for  $N = 2000$  and  $a/a_{HO} = 4.33 \times 10^{-3}$ . We note that there are differences between the full solution of equation (8) and that using the Lieb *et al* [23] approximation for the interaction term. The

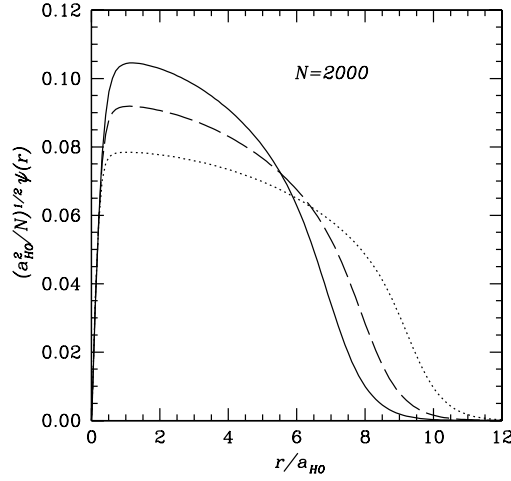


**Figure 3.** (a) The vortex state wavefunction  $\psi(r)$  as a function of the radial distance for a system of  $N = 2000$  atoms and  $a/a_{HO} = 4.33 \times 10^{-3}$ . The solid and dotted curves indicate calculations using the mean-field equation with  $\ln |\psi|^2 a^2$  and  $\ln |\bar{\rho} a^2$  factors, respectively. (b) The core region of the vortex state wavefunction  $\psi(r)$  as a function of the radial distance for a system of  $N = 2000$  atoms and  $a/a_{HO} = 4.33 \times 10^{-3}$ . The solid and dotted curves indicate calculations using the mean-field equation with  $\ln |\psi|^2 a^2$  and  $\ln |\bar{\rho} a^2|$  factors, respectively.

size of the vortex core is typically given by the healing (or coherence) length  $\xi$ , which can be obtained from the balance between the interaction and kinetic energies. Replacing the central density by the average TF density, we obtain  $\xi/a_{HO} = [3 \ln(N^{1/2}(a/a_{HO})^2/3\pi)/8n^{1/2}]^{1/2}$  for the vortex core radius. In figure 3(b), the small- $r$  region of the vortex wavefunction is plotted. We observe that  $\xi/a_{HO} \approx 0.28$  for  $N = 2000$  and  $a/a_{HO} = 4.33 \times 10^{-3}$  correctly describes the size of the vortex core region. We also find that the approximate form of the interaction  $\sim |\ln \bar{\rho} a^2|$  does not affect the vortex wavefunction in the core region.

Recent experiments by Cornish *et al* [37] have demonstrated the feasibility of tuning the scattering length of atomic gases through Feshbach resonances. This opens the possibility of studying the effects of those interactions and regimes described beyond the GP equation more systematically. To understand how the condensate wavefunction with a vortex is affected by the





**Figure 4.** The vortex state  $\psi(r)$  as a function of the radial distance for a system of  $N = 2000$  atoms, at different values of the hard-disc radius  $a$ . The dotted, dashed and solid curves correspond to  $a/a_{HO} = 5 \times 10^{-2}$ ,  $10^{-2}$  and  $5 \times 10^{-3}$ , respectively.

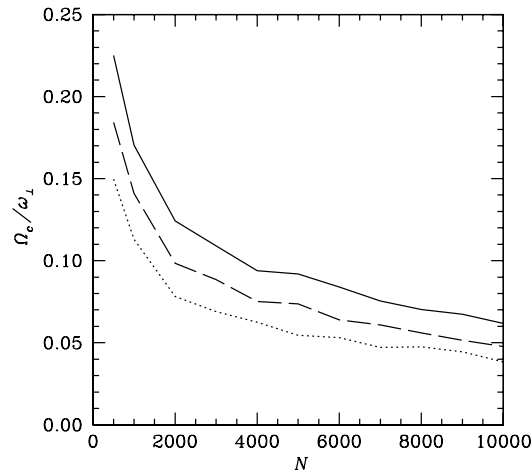
interaction strength (i.e. hard-disc radius  $a$ ) we display in figure 4 the solution of equation (8) for three different values of  $a$ . We observe that for a fixed number of particles, as  $a$  increases, the vortex wavefunction is depleted in the middle region and is extended to a larger spatial region. Interestingly, the core region seems largely unaffected by the interaction strength. This is because the vortex size depends logarithmically on the scattering length  $a$ . For the chosen values of  $a$  in figure 4 the diluteness condition  $\rho a^2/|\ln \rho a^2| \ll 1$  is fulfilled so equation (8) should provide an adequate description. For much larger values of  $N$  and  $a$ , it may be necessary to include the higher-order corrections provided by the perturbative results for homogeneous 2D bosons.

We also calculate the critical angular frequency to produce a vortex state using the energy difference formula [33]

$$\Omega_c = \frac{1}{\kappa} [(E/N)_\kappa - (E/N)_0], \quad (9)$$

where we compare the energy of a vortex state in the frame rotating with angular frequency  $\Omega$ , namely,  $E - \Omega L_z$ , with the ground state energy without vortices. Since angular momentum  $L_z$  per particle is simply  $\hbar \kappa$ ,  $\Omega_c$  gives the critical value of the angular frequency for the formation of a vortex. Figure 5 shows that  $\Omega_c$  decreases with increasing  $N$ . Note, however, for large  $N$  the vortex core radius decreases. Therefore, the optimal value of  $N$  required to observe vortices is not very large. It is also interesting to find that the formation of vortices becomes easier (smaller values of  $\Omega_c$  are required) with increasing interaction strength (larger  $a$ ).

In summary, we have considered the ground state properties of 2D Bose condensates at zero temperature within a mean-field description. In contrast to the 3D case and some models of the Q2D case, in two dimensions the interaction term depends logarithmically on the scattering length and condensate density. We have solved the GP equation describing the 2D condensate numerically and compared the results with other models. We have found that the local-density approximation based approach, without any adjustable parameters, can be useful in identifying the strictly 2D limit of condensates by tuning the asymmetry parameter experimentally. We have also investigated the vortex states in such condensates by introducing a complex phase in the wavefunction. Increasing the interaction strength favours the formation



**Figure 5.** The critical frequency of rotation for the vortex formation in 2D condensates for various interaction strengths. The dotted, dashed and solid curves are for the scattering lengths  $a/a_{\text{HO}} = 5 \times 10^{-2}$ ,  $10^{-2}$  and  $10^{-3}$ , respectively.

of vortices. It would be interesting to extend the calculations presented here to study finite temperature effects, especially in connection with the superfluid properties of the system. The role of the  $|\ln \psi^2 a^2|^{-1}$  correction to the GP equation and the interaction with non-condensed thermal particles awaits a separate study. In order to understand the significance of interactions and high-density effects better precision Monte Carlo simulations would be useful as a test of the range of validity of the mean-field and local-density approximations.

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